# Multi-Frequency Phase Synchronization

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# Outline

**Motivation**

- Synchronization
- Geometric Model of Fibre Bundles

Multi-Frequency Phase Synchronization

- Phase Synchronization
- Multi-Frequency Formulation
- Theory

Application to Multi-Frequency Class Averaging

Joint work with **Zhizhen Zhao (UIUC)**

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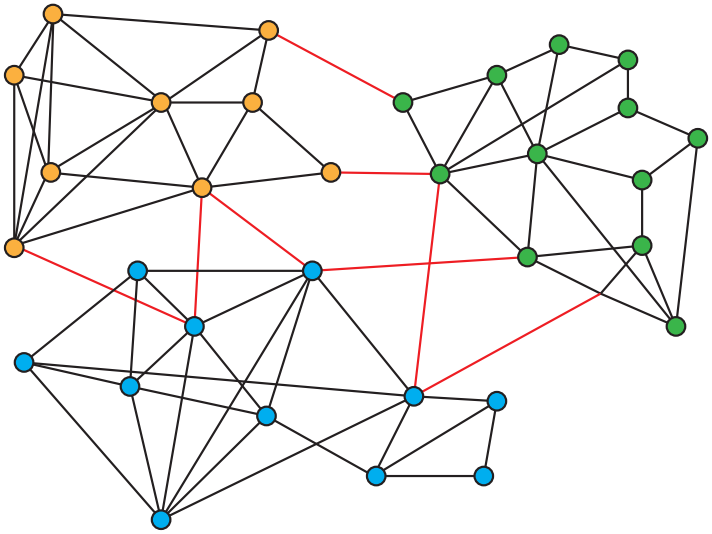
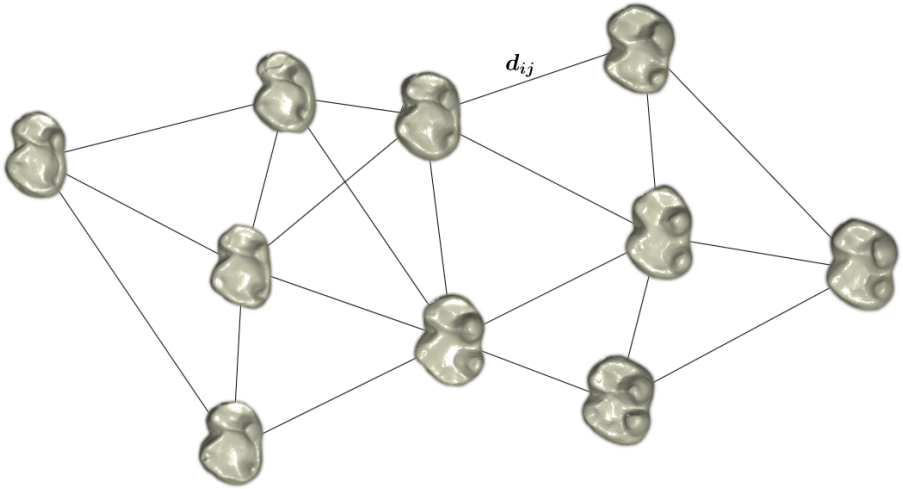
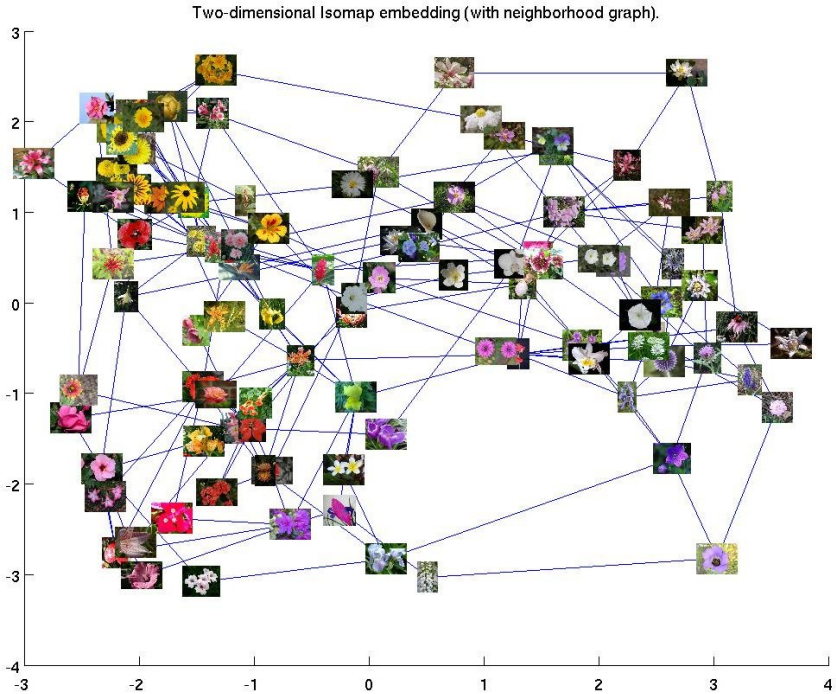
# Graph-Based Data Analysis



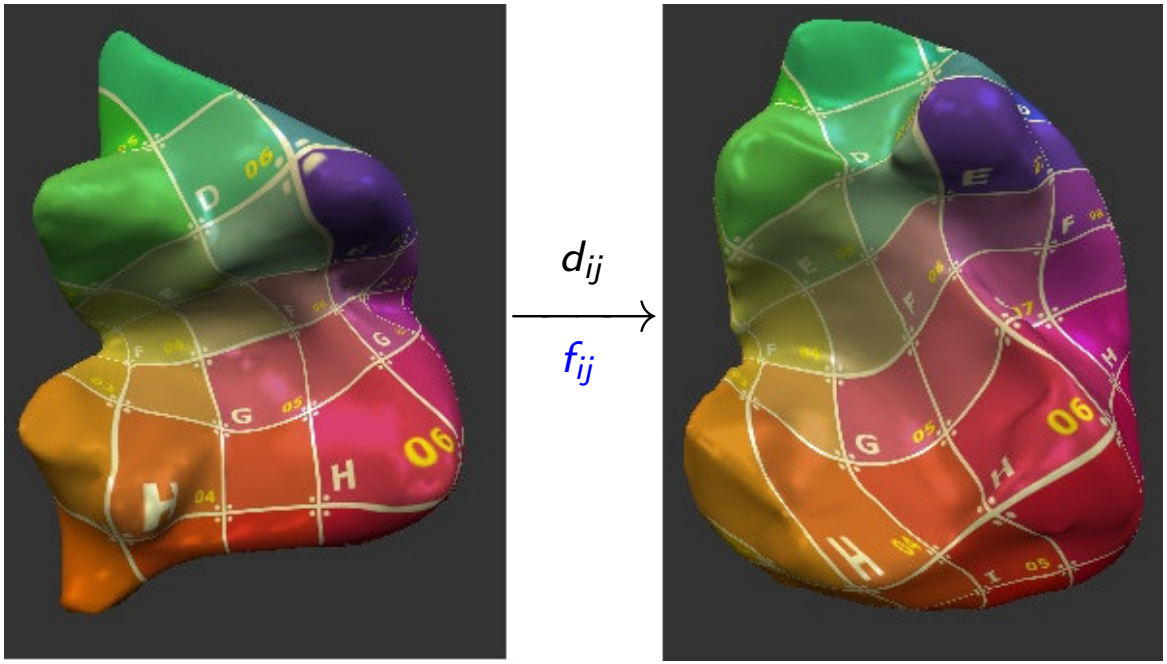


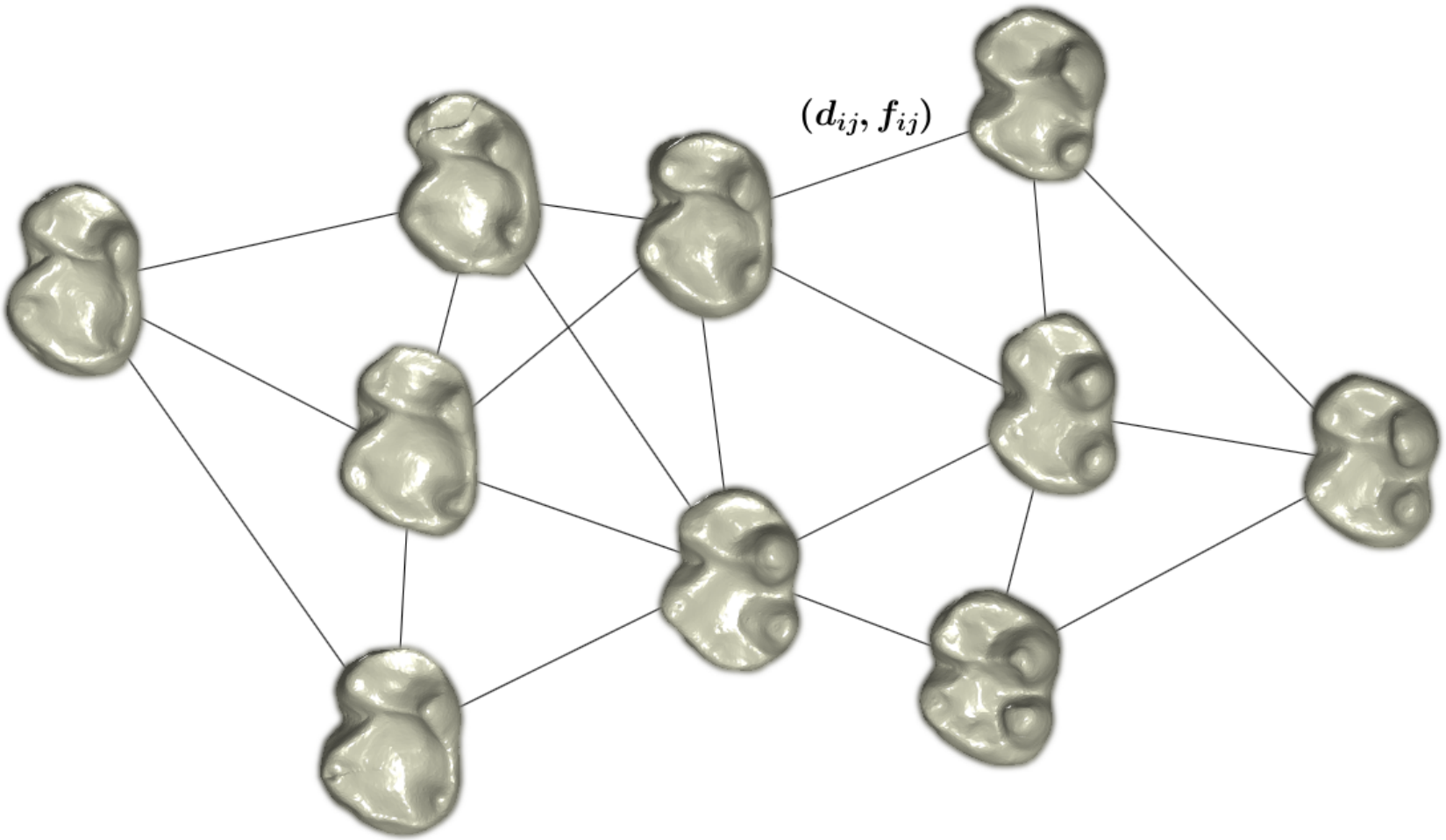
# Evolutionary Biology

$$d_{\mathrm{cP}}\left(S_i, S_j\right) = \inf_{\mathcal{C}\in\mathcal{A}\left(S_i,S_j\right)} \inf_{R\in\mathbb{E}(3)} \left(\int_{S_i} \left\|R\left(x\right) - \mathcal{C}\left(x\right)\right\|^2 d\mathrm{vol}_{S_i}\left(x\right)\right)^{\frac{1}{2}}$$

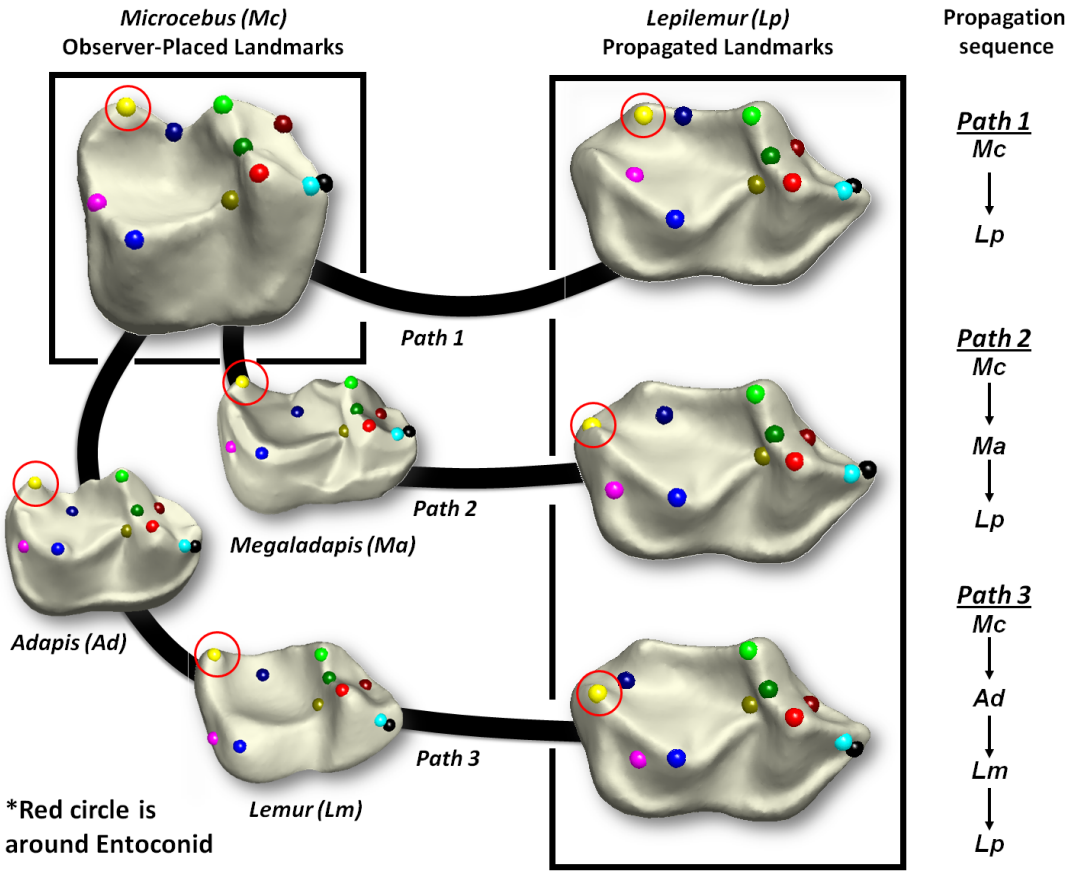
$S_i$




$S_j$

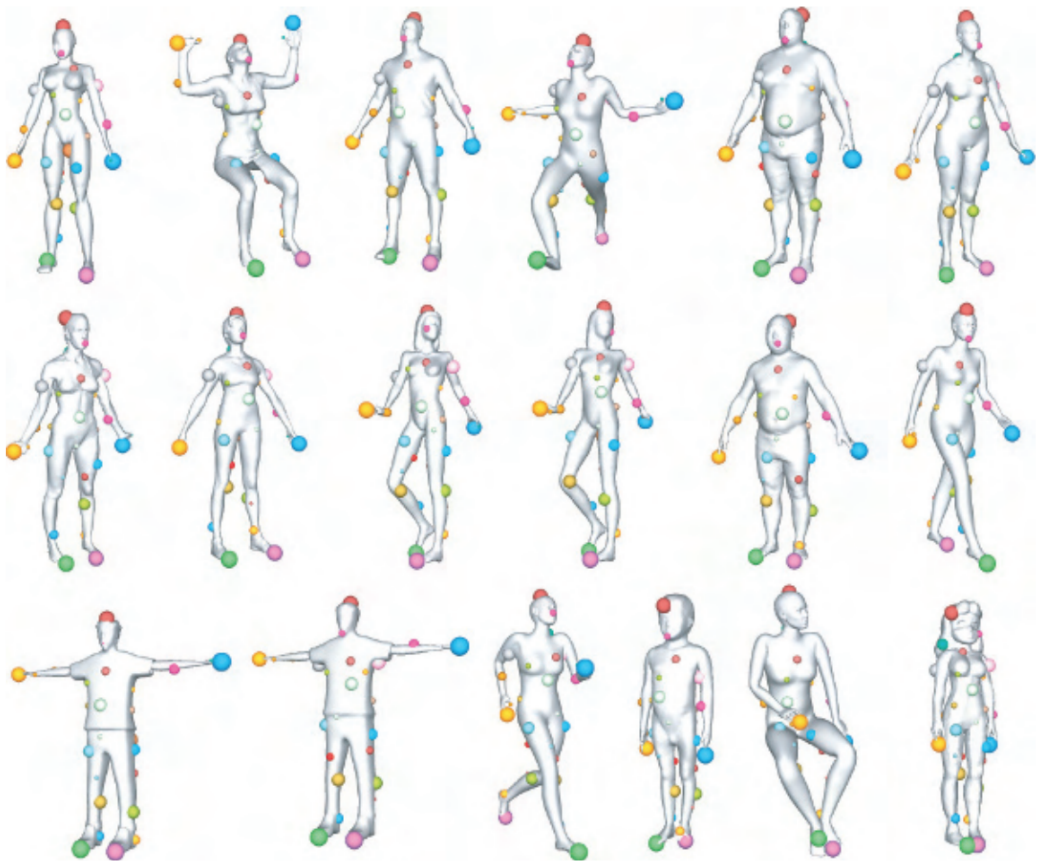

$(d_{ij}, f_{ij})$

# Interpretability Issue



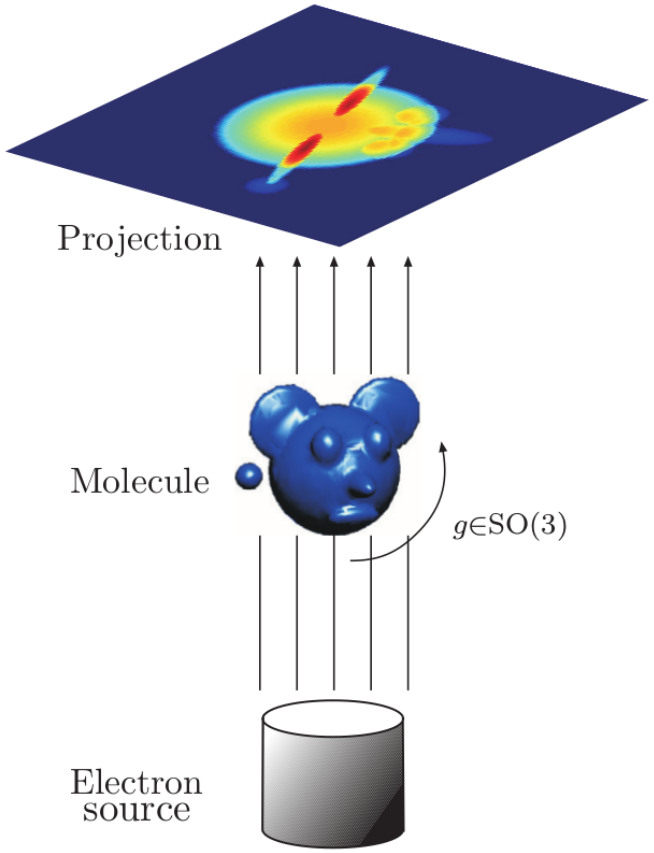

• Boyer et al. "Algorithms to Automatically Quantify the Geometric Similarity of Anatomical Surfaces." *Proceedings of the National Academy of Sciences* 108.45 (2011): 18221–18226.

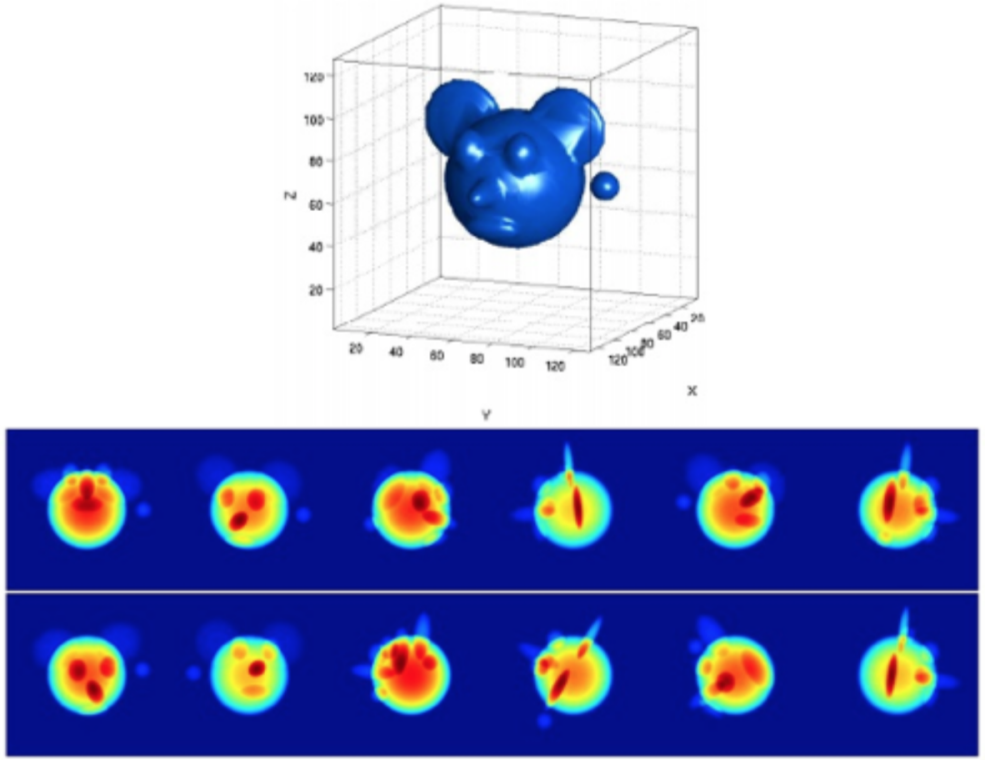
# Collection Shape Analysis



• Q. Huang & L. Guibas. "Consistent Shape Maps via Semidefinite Programming", *Computer Graphics Forum*, vol. 32, no. 5, pp. 177–186 (2013).

# Cryo-Electron Microscopy



• Singer et al. "Viewing Angle Classification of Cryo-Electron Microscopy Images using Eigenvectors", *SIAM Journal on Imaging Sciences*, 4 (2), pp. 543–572 (2011).

# Cryo-Electron Microscopy: Real Challenge is Low SNR

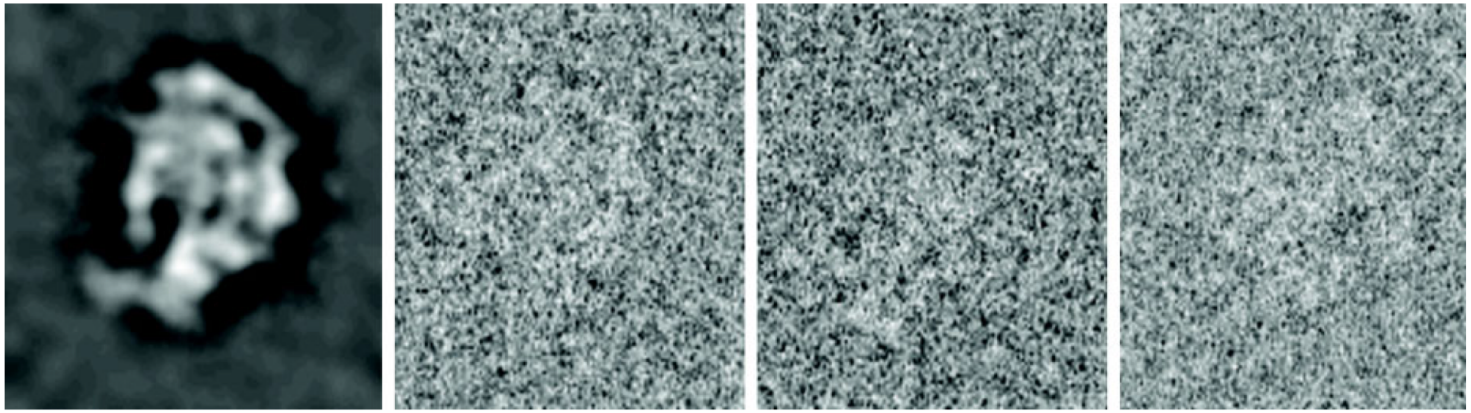
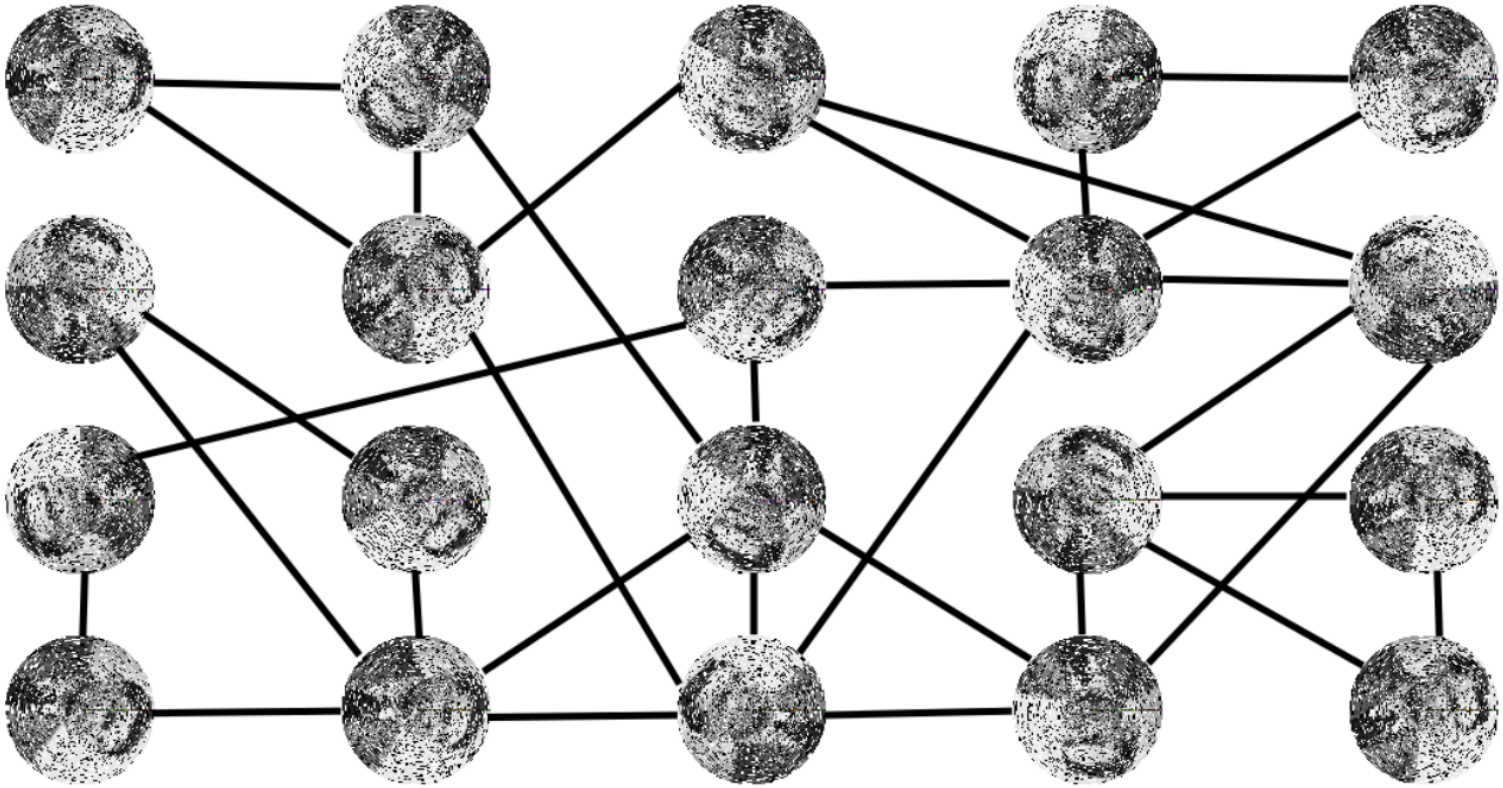


**Fig. 3** The left most image is a clean simulated projection image of the E.coli 50S ribosomal subunit. The other three images are real electron microscope images of the same subunit

• Hadani & Singer. "Representation Theoretic Patterns in Three-Dimensional Cryo-Electron Microscopy II – The Class Averaging Problem," *Foundations of Computational Mathematics*, 11 (5), pp. 589–616 (2011).

$$y_i = R_i x + \xi_i$$
$$R_i \in O(d), \quad \xi_i \sim \text{i.i.d. noise}$$



- Afonso S. Bandeira. "Ten Lectures and Forty-Two Open Problems in the Mathematics of Data Science." (2015).

$$\boxed{\begin{array}{c} y_i = R_i x + \xi_i \\ R_i \in O(d), \quad \xi_i \sim \text{i.i.d. noise} \end{array}}$$

$$\begin{aligned} \text{Measurement:} \quad & R_{ij} \approx R_i^\top R_j \\ \text{Recover:} \quad & R_1, R_2, \cdots \end{aligned}$$

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$\Rightarrow$ Solve the minimization problem

$$\min_{R_1, R_2, \cdots \in O(d)} \quad \sum_{(i,j) \in E} w_{ij} \left\| R_{ij} - R_i^\top R_j \right\|_{\mathrm{F}}^2$$

$$\frac{1}{2} \sum_{1 \leq i,j \leq N} w_{ij} \left\| R_{ij} - R_i^\top R_j \right\|_{\mathrm{F}}^2$$

$$
\begin{aligned}
&\frac{1}{2}\sum_{1\le i,j\le N} w_{ij}\left\|R_{ij}-R_i^\top R_j\right\|_{\mathrm{F}}^2 \\
&\quad=\frac{1}{2}\sum_{1\le i,j\le N} w_{ij}\mathrm{Tr}\left[\left(R_i^\top-R_{ij}R_j^\top\right)\left(R_i-R_jR_{ij}^\top\right)\right] \\
&\quad=\sum_{1\le i,j\le N} w_{ij}\mathrm{Tr}\left(I_{d\times d}-R_iR_{ij}R_j^\top\right)
\end{aligned}
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&\quad=\sum_{1\le i,j\le N} w_{ij}\mathrm{Tr}\left(I_{d\times d}-R_iR_{ij}R_j^\top\right) \\
&\quad=\mathrm{Tr}\left(\left[R_1,\cdots,R_N\right]\left(\mathscr{D}-\mathscr{W}\right)\begin{bmatrix}R_1^\top\\ \vdots\\ R_N^\top\end{bmatrix}\right)
\end{aligned}
$$

where

$$
\mathscr{D}=\begin{bmatrix} d_1 I_{d\times d} & & \\ & \ddots & \\ & & d_N I_{d\times d}\end{bmatrix},\mathscr{W}=\begin{bmatrix} w_{11}R_{11} & \cdots & w_{1N}R_{1N}\\ \vdots & & \vdots\\ w_{N1}R_{N1} & \cdots & w_{NN}R_{NN}\end{bmatrix}
$$

# QO-OC

$$\min_{R_1,R_2,\cdots\in O(d)} \quad \sum_{(i,j)\in E} w_{ij} \left\| R_{ij} - R_i^\top R_j \right\|_{\mathrm{F}}^2$$

$$\Leftrightarrow \quad \min_{R_1,\cdots,R_N\in\mathbb{R}^{d\times d}} \mathrm{Tr}\left( \left[R_1,\cdots,R_N\right] \left(\mathscr{D}-\mathscr{W}\right) \begin{bmatrix} R_1^\top \\ \vdots \\ R_N^\top \end{bmatrix} \right)$$

$$\text{s.t.} \qquad R_1^\top R_1 = \cdots = R_N^\top R_N = I_{d\times d}$$

• A. Nemirovski, "Sums of Random Symmetric Matrices and Quadratic Optimization Under Orthogonality Constraints", *Math. Programming*, 109 (2007), pp. 283–317.

# Convex Relaxations (I)

$$\min_{R_1,\cdots,R_N \in \mathbb{R}^{d\times d}} \operatorname{Tr}\left( \left[R_1, \cdots, R_N\right] \left(\mathscr{D} - \mathscr{W}\right) \begin{bmatrix} R_1^\top \\ \vdots \\ R_N^\top \end{bmatrix} \right)$$
$$\text{s.t.} \qquad R_1^\top R_1 = \cdots = R_N^\top R_N = I_{d\times d}$$

- Spectral Relaxation

$$\boxed{\begin{aligned} &\min_{\mathcal{R} \in \mathbb{R}^{d\times Nd}} \operatorname{Tr}\left(\mathcal{R}\left(\mathscr{D} - \mathscr{W}\right)\mathcal{R}^\top\right) \\ &\text{s.t.} \qquad \mathcal{R}\mathcal{R}^\top = N \cdot I_{d\times d} \end{aligned}}$$

• Chaudhury et al. "Global Registration of Multiple Point Clouds using Semidefinite Programming", *SIAM Journal on Optimization*, 25(1):468–501, 2015.

# Convex Relaxations (II)

$$\min_{R_1,\cdots,R_N \in \mathbb{R}^{d\times d}} \operatorname{Tr}\left( (\mathscr{D} - \mathscr{W}) \begin{bmatrix} R_1^\top \\ \vdots \\ R_N^\top \end{bmatrix} \begin{bmatrix} R_1, \cdots, R_N \end{bmatrix} \right)$$
$$\text{s.t.} \qquad R_1^\top R_1 = \cdots = R_N^\top R_N = I_{d\times d}$$

- 

$$\boxed{\begin{aligned} \min_{\mathcal{G} \in \mathbb{R}^{Nd\times Nd}} \quad & \operatorname{Tr}\left( (\mathscr{D} - \mathscr{W})\, \mathcal{G} \right) \\ \text{s.t.} \quad & \mathcal{G} \succeq 0,\ \mathcal{G} = \mathcal{G}^\top \\ & \mathcal{G}_{ii} = I_{d\times d},\ 1 \le i \le N \\ & \operatorname{rank}(\mathcal{G}) = d \end{aligned}}$$

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- SDP Relaxation

$$\boxed{\begin{aligned} \min_{\mathcal{G} \in \mathbb{R}^{Nd\times Nd}} \quad & \operatorname{Tr}\left( (\mathscr{D} - \mathscr{W})\, \mathcal{G} \right) \\ \text{s.t.} \quad & \mathcal{G} \succeq 0,\ \mathcal{G} = \mathcal{G}^\top \\ & \mathcal{G}_{ii} = I_{d\times d},\ 1 \le i \le N \\ & \cancel{\operatorname{rank}(\mathcal{G}) = d} \end{aligned}}$$

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# Synchronization Problems

- Data:
  - graph $\Gamma = (V, E)$
  - topological group $G$, equipped with a norm $\|\cdot\|$, and a $G$-module $F$
  - **edge potential** $\rho : E \to G$ satisfying $\rho_{ij} = \rho_{ji}^{-1}$, $\forall (i,j) \in E$
- Goal:
  - find a **vertex potential** $f : V \to G$ or $F$ such that

$$f_i = \rho_{ij} f_j, \quad \forall (i,j) \in E$$

- The goal can be achieved if and only if $\rho_{ij} = f_i f_j^{-1}$
- **Not** always feasible!

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- The goal can be achieved if and only if $\rho_{ij} = f_i f_j^{-1}$
- **Not** always feasible!
- If infeasible, find the "closest solution" in the sense of

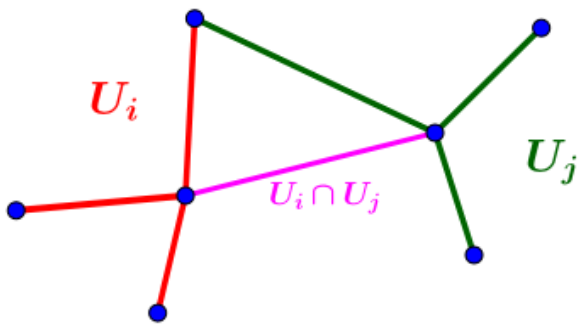
$$\min_{\substack{f:V\to G \\ \|f\|\neq 0}} \frac{1}{2} \frac{\sum_{i,j\in V} \|f_i - \rho_{ij} f_j\|^2}{\sum_{i\in V} \|f_i\|^2} (=: \eta(f))$$

# Synchronization Problems: Examples

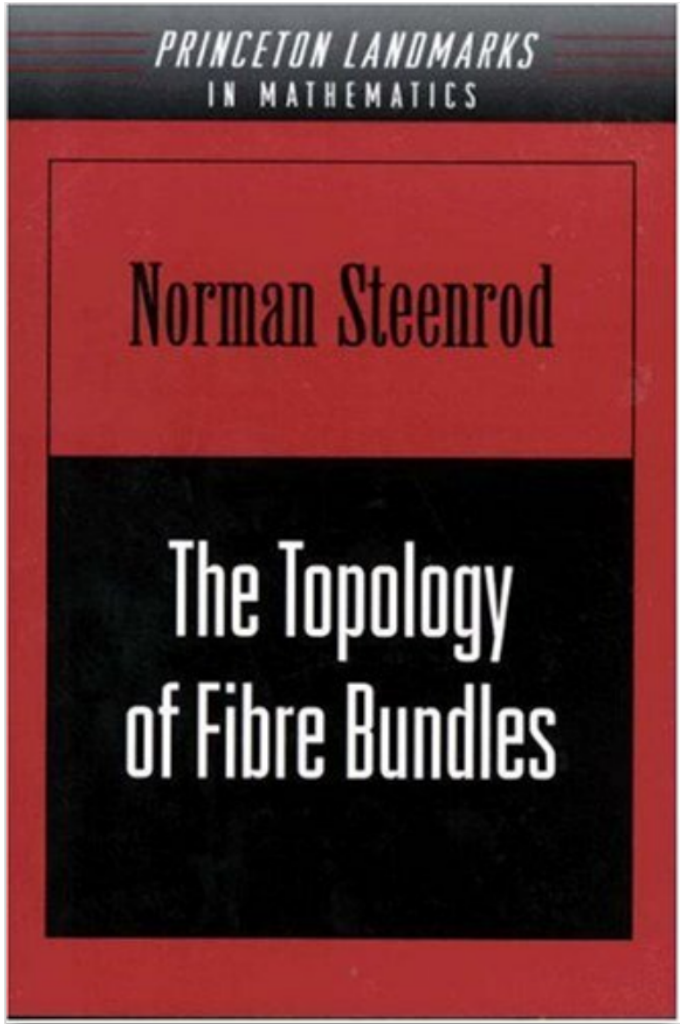
- Manifold Orientability [Singer, Wu (2011)]: $G = O(1)$
- Angular Synchronization [Singer (2011)]: $G = U(1)$
- Vector Diffusion Maps [Singer, Wu (2012)]: $G = O(d)$
- Multireference Alignment [Bandeira et al. (2014)]: $G = \{\text{cyclic shifts}\}$
- Global Registration of Point Clouds [Chaudhury (2015)]: $G = \mathbb{E}_d$
- Collection Shape Matching [Nguyen et al. (2011)], [Huang, Guibas (2013)], [Chen et al. (2014)], [Maron et al. (2016)]: $G = \text{permutation group}$
- Cryo-EM Structural Reconstruction [Singer et al. (2011)], [Shkolnisky, Singer (2012)], [Zhao, Singer (2014)], [Bandeira et al. (2015)]: $G = SO(3)$

# The Geometry of Synchronization Problems

- Data:
  - graph $\Gamma = (V, E)$
  - topological group $G$, equipped with a norm $\|\cdot\|$, and a $G$-module $F$
  - **edge potential** $\rho : E \to G$ satisfying $\rho_{ij} = \rho_{ji}^{-1}$, $\forall (i,j) \in E$
- Flat Principal Bundle:
  - Let $\mathfrak{U} = \{U_i \mid 1 \leq i \leq |V|\}$ be an open cover of $\Gamma$ (viewed as a 1-dimensional simplicial complex), where $U_i$ is the *(open) star neighborhood* of vertex $i$.



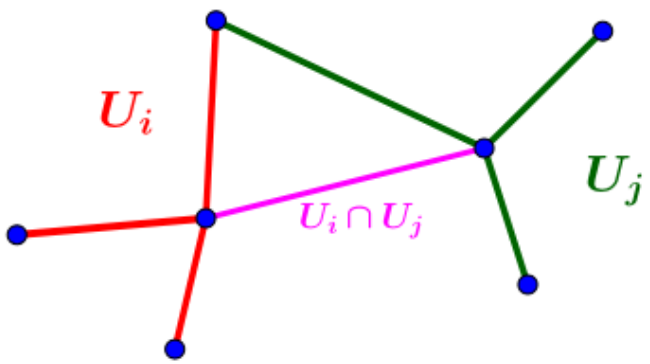

  - Triplet $(\rho, G, \Gamma)$ defines a *flat principal $G$-bundle* $\mathscr{B}_\rho$ over $\Gamma$




**Theorem** (Steenrod 1951, §2). If topological group $G$ acts on $Y$ and $\{U_i\}$, $\{g_{ij}\}$ is a system of coordinate transformations in the space $X$ such that

$$\begin{aligned} g_{ii} &= e \in G \quad \text{for all } U_i \\ g_{ij} &= g_{ji}^{-1} \quad \text{if } U_i \cap U_j \neq \emptyset \\ g_{ij} g_{jk} &= g_{ik} \quad \text{if } U_i \cap U_j \cap U_k \neq \emptyset \end{aligned}$$

then there exists a fibre bundle $\mathscr{B}$ with base space $X$, fibre $Y$, group $G$, and coordinate transforms $\{g_{ij}\}$.




**No triple intersections!**

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then there exists a fibre bundle $\mathscr{B}$ with base space $X$, fibre $Y$, group $G$, and coordinate transforms $\{g_{ij}\}$.

# Geometric Observations

- Denote

$$C^0(\Gamma; G) := \{f : V \to G\}$$
$$C^1(\Gamma; G) := \left\{\rho : E \to G \mid \rho_{ij} = \rho_{ji}^{-1}, \forall (i,j) \in E\right\}$$

- Consider the right action of $C^0(\Gamma; G)$ on $C^1(\Gamma; G)$:

$$\begin{aligned} C^1(\Gamma; G) \times C^0(\Gamma; G) &\to C^1(\Gamma; G) \\ (\rho, f) &\longmapsto \tau_\rho f \end{aligned}$$

  defined as $(\tau_f \rho)_{ij} := f_i^{-1} \rho_{ij} f_j, \quad \forall (i,j) \in E$. Denote the orbit space of $\tau_f$ by $C^1(\Gamma; G) / C^0(\Gamma; G)$

- $\rho$ synchronizable $\Leftrightarrow$ $\tau_f \rho$ synchronizable for all $f \in C^0(\Gamma; G)$, i.e. synchronizability is defined up to orbits of $\tau_f$

# Moduli Space of Synchronization Data

**Theorem (G. et al. 2019).** There exists a one-to-one correspondence (between *sets*)

$$C^1(\Gamma; G) / C^0(\Gamma; G) \cong \mathrm{Hom}(\pi_1(\Gamma), G) / G$$

where $G$ acts on $\mathrm{Hom}(\pi_1(\Gamma), G)$ by conjugations:

$$\begin{aligned} \mathrm{Hom}(\pi_1(\Gamma), G) \times G &\longrightarrow \mathrm{Hom}(\pi_1(\Gamma), G) \\ (\phi, g) &\longmapsto g^{-1}\phi g \end{aligned}$$

• Tingran Gao, Jacek Brodzki, Sayan Mukherjee. "The Geometry of Synchronization Problems and Learning Group Actions." *Discrete & Computational Geometry*, to appear (2019) arXiv:1610.09051

$$C^1(\Gamma; G) / C^0(\Gamma; G) \cong \mathrm{Hom}(\pi_1(\Gamma), G) / G$$

- **LHS**: The *first cohomology set* $\check{H}^1((\Gamma, \mathfrak{U}), \underline{G})$
- **RHS**: The *representation variety* of $\pi_1(\Gamma)$ with value in $G$
- Proof builds upon construction of a *holonomy homomorphism*
- In particular, $\rho \in C^1(\Gamma; G)$ synchronizable
  $\Leftrightarrow [\rho] = [e]$ as equivalence classes in $C^1(\Gamma; G) / C^0(\Gamma; G)$
  $\Leftrightarrow$ the principal $G$-bundle $\mathscr{B}_\rho$ is trivial

# Learning Group Actions by Synchronization

## Problem (Learning Group Actions by Synchronization)

*Denote $\mathscr{X}_K$ for all partitions of $\Gamma$ into $K$ nonempty connected components ($K \leq n$) and*

$$\nu\left(S_i\right) = \inf_{f \in C^0(\Gamma;G)} \sum_{j,k \in S_i} w_{jk} \left\| f_j - \rho_{jk} f_k \right\|^2, \ \mathrm{vol}\left(S_i\right) = \sum_{j \in S_i} d_j,$$

*Solve the optimization problem*

$$\min_{\{S_1,\cdots,S_K\} \in \mathscr{X}_K} \frac{\max\limits_{1 \leq i \leq K} \nu\left(S_i\right)}{\min\limits_{1 \leq i \leq K} \mathrm{vol}\left(S_i\right)} \tag{1}$$

*and output an optimal partition $\{S_1, \cdots, S_K\}$ together with the minimizing $f \in C^0\left(\Gamma; G\right)$.*

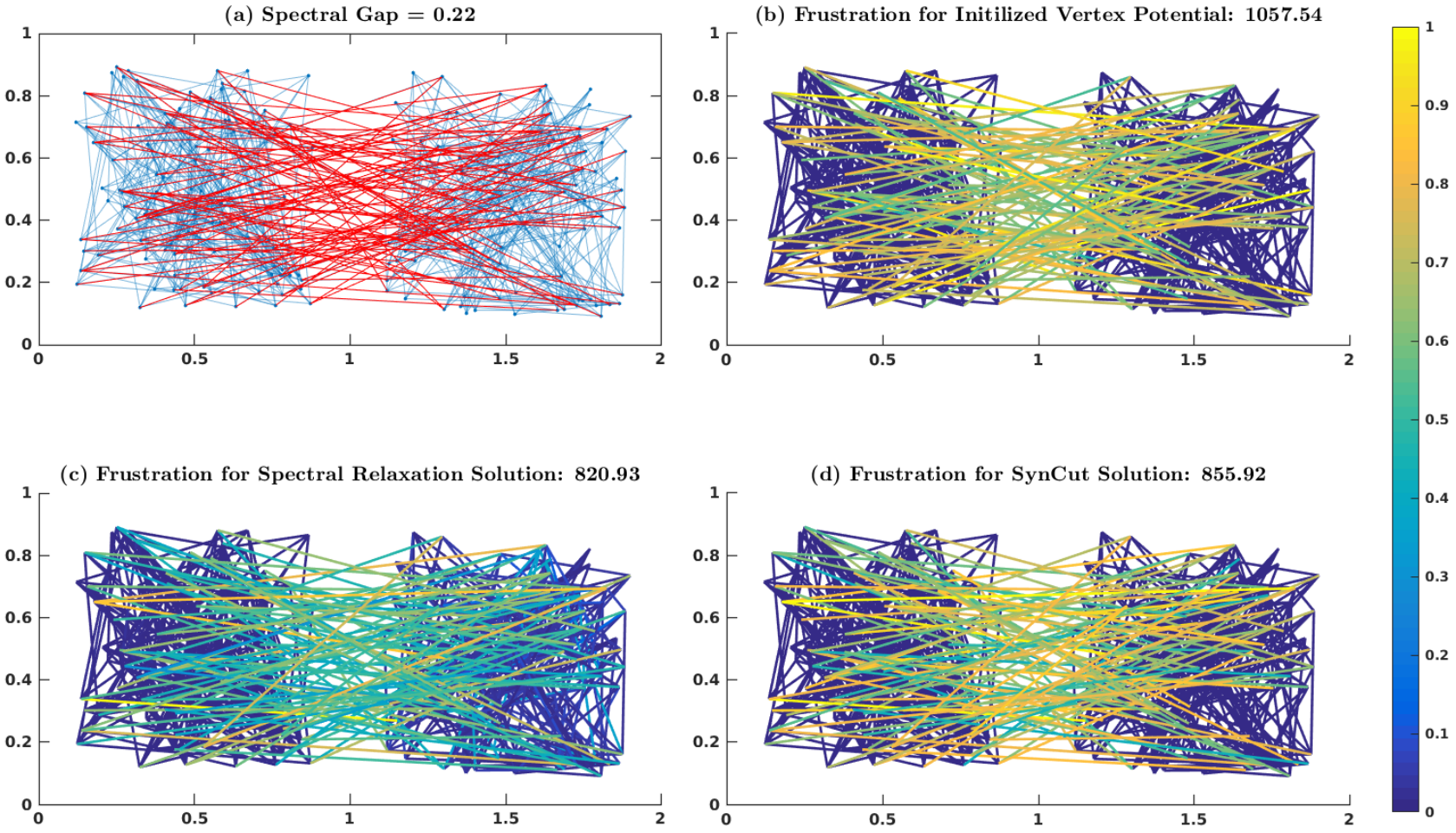
# Algorithm: SynCut

Input: $\Gamma = (V, E, w)$, $\rho \in C^1(\Gamma; G)$, number of partitions $K$
Output: Partitions $\{S_1, \cdots, S_K\}$

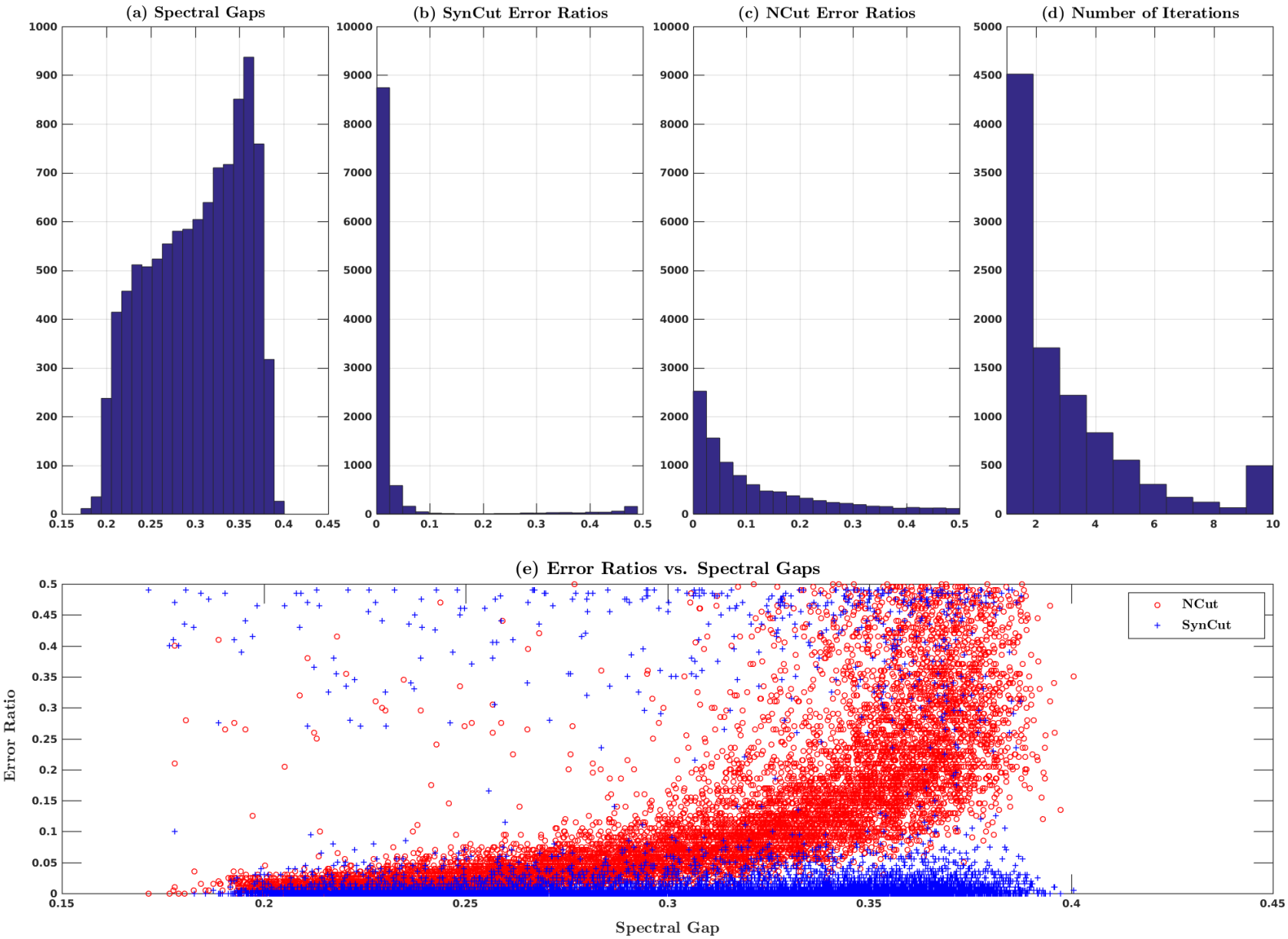
1. Solve synchronization problem over $\Gamma$ for $\rho$, obtain $f \in C^0(\Gamma; G)$
2. Compute $d_{ij} = \exp\left(-w_{ij} \|f_i - \rho_{ij} f_j\|^2\right)$ on all edges $(i, j) \in E$
3. Spectral clustering on weighted graph $(V, E, d)$ to get $\{S_1, \cdots, S_k\}$
4. Solve synchronization problem within each partition $S_j$, "glue up" the local solutions to obtain $f_* \in C^0(\Gamma; G)$
5. $f \leftarrow f_*$, repeat from Step 2


• Tingran Gao, Jacek Brodzki, Sayan Mukherjee. "The Geometry of Synchronization Problems and Learning Group Actions." *Discrete & Computational Geometry,* to appear (2019) arXiv:1610.09051
• Chandrajit Bajaj, Tingran Gao, Zihang He, Qixing Huang, and Zhenxiao Liang. "SMAC: Simultaneous Mapping and Clustering Using Spectral Decompositions." *Proceedings of the 35th International Conference on Machine Learning,* PMLR 80:324–333, 2018.

# Clustering based on Synchronization Residuals



# Compare with Spectral Clustering



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# Phase Synchronization: Synchronization Over $\mathrm{U}(1)$

- Assume the underlying graph $\Gamma$ is complete
- **Ground truth**: phase vector $z = (\exp \iota\theta_1, \ldots, \exp \iota\theta_n)^\top \in \mathbb{C}_1^n$
- **Measurements**: *noisy* pairwise phase offsets $H_{ij} \approx z_i \bar{z}_j$, or in matrix form

$$H := zz^* + \mathrm{noise}$$

- **Goal**: recover the true phase vector $z$ (up to a global multiplicative factor)
- **Spectral Relaxation**: solve for the top eigenvector of $H$, denoted as $\tilde{x}$ (scaled to $\|\tilde{x}\|_2 = \sqrt{n}$), then define $\hat{x} \in \mathbb{C}_1^n$ by

$$\hat{x}_i := \tilde{x}_i / |\tilde{x}_i|$$

# Noise Models

- **Additive Gaussian Noise Model**

$$H = zz^* + \sigma W$$

where $W$ is a standard complex Wigner matrix with i.i.d. standard complex Gaussian entries above the diagonal

- **Random Corruption Model**

$$H_{ij} = \begin{cases} z_i \bar{z}_j & \text{with prob. } r \in [0,1] \\ \mathrm{Unif}\,(\mathrm{U}(1)) & \text{with prob. } 1-r \end{cases}$$

# Optimization Problem Formulation

$$\min_{x \in \mathbb{C}_1^n} \|xx^* - H\|_{\mathrm{F}}^2 \quad \Leftrightarrow \quad \max_{x \in \mathbb{C}_1^n} x^* H x$$

- We may well assume $z = (1, \ldots, 1)^\top$
- Nonconvex problem, can be attacked using convex (spectral or SDP) relaxation
- For additive Gaussian noise, convex relaxation almost recovers the ground truth $z \in \mathbb{C}_1^n$ with high probability for noise level up to $\sigma = O\left(\sqrt{n/\log n}\right)$ **[Zhong & Boumal (2018)]**; non-rigorous statistical-physics-based methods predict the same holds up to $\sigma = O\left(\sqrt{n}\right)$ **[Javanmard et al. (2016)]**
- For random corruption model, **[Singer (2011)]** argues that $|\mathrm{Corr}\,(\tilde{x}, z)| > 1/\sqrt{n}$ with high probability if $r > 1/\sqrt{n}$

# Outline


Motivation

- Synchronization
- Geometric Model of Fibre Bundles

**Multi-Frequency Phase Synchronization**

- Phase Synchronization
- **Multi-Frequency Formulation**
- Theory

Application to Multi-Frequency Class Averaging


Joint work with **Zhizhen Zhao (UIUC)**

# Multi-Frequency Phase Synchronization

- Assume random corruption model
- Instead of solving

$$\max_{x \in \mathbb{C}_1^n} x^* H x$$

  let us solve

$$\boxed{\max_{x \in \mathbb{C}_1^n} \sum_{k=1}^{k_{\max}} (x^k)^* H^{(k)} x^k}$$

  where $x^k := \left(x_1^k, \ldots, x_n^k\right)^\top \in \mathbb{C}_1^n$, and $H^{(k)}$ is the $n$-by-$n$ Hermitian matrix with $H_{ij}^{(k)} := H_{ij}^k$
- Solving this nonconvex optimization by a popular two-stage strategy: (i) produce a good initialization (ii) perform local methods e.g. gradient descent or (generalized) power iteration

• Tingran Gao & Zhizhen Zhao. "Multi-Frequency Phase Synchronization," *The 36th International Conference on Machine Learning* (ICML 2019). arXiv:1901.08235.

# Multi-Frequency Phase Synchronization: Stage 1

- Fix $k_{\max} \geq 1$, build $H^{(2)}, \ldots, H^{(k_{\max})}$ out of $H = H^{(1)}$
- For each $k = 1, \ldots, k_{\max}$, solve the subproblem

$$u^{(k)} := \arg\max_{v \in \mathbb{C}_1^n} \; v^* H^{(k)} v$$

  using any convex relaxation, and set $W^{(k)} := u^{(k)} \left(u^{(k)}\right)^*$
- For all $1 \leq i, j \leq n$, find the "peak location" of the spectrogram

$$\hat{\theta}_{ij} := \arg\max_{\phi \in [0, 2\pi]} \left| \mathrm{Re} \left\{ \sum_{k=1}^{k_{\max}} W_{ij}^{(k)} e^{-\iota k \phi} \right\} \right|$$

- Construct Hermitian matrix $\widehat{H} \in \mathbb{C}_1^{n \times n}$ by $\widehat{H}_{ij} = \exp \iota \hat{\theta}_{ij}$, extract the top eigenvector $\tilde{x}$, and perform entrywise normalization to get $\hat{x} \in \mathbb{C}_1^n$

# Multi-Frequency Phase Synchronization: Stage 2

Basically do generalized power iteration, but with a little extra work to ensure the $k_{\max}$ frequency channels "march in formation"

- For iteration counter $t = 0$, set $z^{(k,0)} := \hat{x}^k$ for $k = 1, \ldots, k_{\max}$
- Until convergence ($t = 1, \ldots, T$),
  - $u^{(k,t)} := H^{(k)} z^{(k,t-1)}$ for $k = 1, \ldots, k_{\max}$
  - For each entry $1 \leq i \leq n$, soft-threshold the spectrogram

$$h_i^{(t)} := \mathrm{Re}\left\{ \sum_{k=1}^{k_{\max}} u_i^{(k,t)} e^{\iota k \theta} \right\}$$

  then convert back

$$\hat{u}_i^{(k,t)} := \int_0^{2\pi} \mathrm{SoftThresh}\left( h_i^{(t)}(\theta) \right) \mathrm{d}\theta$$

  and finally get $z_i^{(k,t)} \in \mathbb{C}_1^n$ by entrywise normalization
- Output $\hat{z} := z^{(1,T)}$

# How does it work? Check correlation $|\mathrm{Corr}\,(\hat{z}, z)|$.....

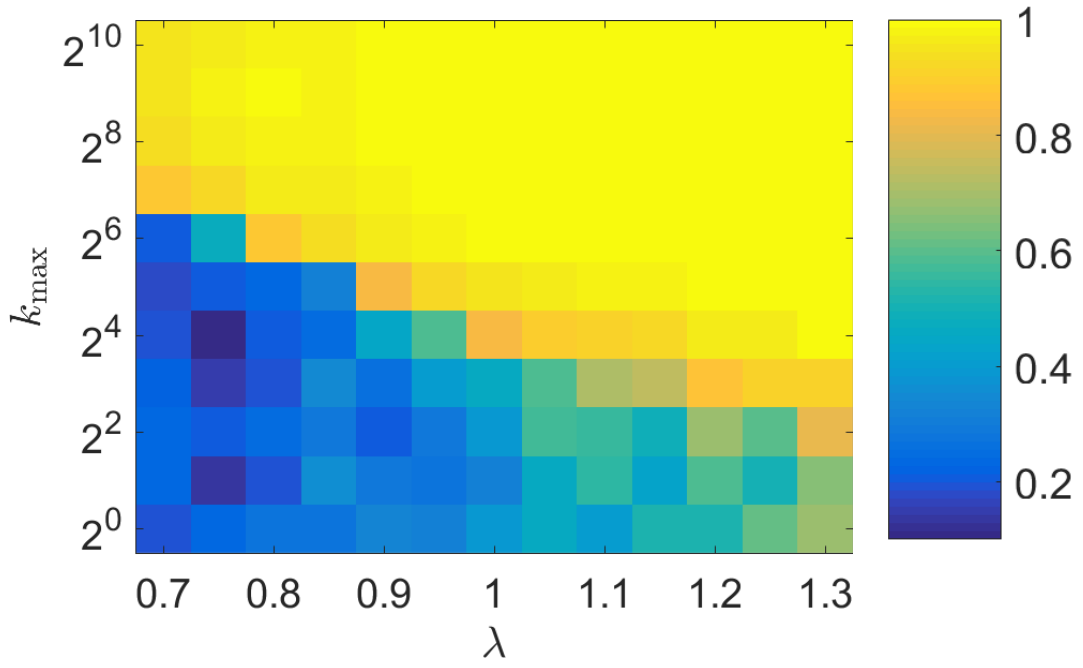


Figure: Random corruption model, $r = \lambda/\sqrt{n}$

- **[Singer (2011)]** only asserts $|\mathrm{Corr}\,(\hat{z}, z)| > 1/\sqrt{n}$ for $\lambda > 1$
- Even for $\lambda < 1$, our method attains $|\mathrm{Corr}\,(\hat{z}, z)| \to 1$ provided that $k_{\max} \gg 1$!

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# Focusing on Stage 1

- Fix $k_{\max} \geq 1$, build $H^{(2)}, \ldots, H^{(k_{\max})}$ out of $H = H^{(1)}$
- For each $k = 1, \ldots, k_{\max}$, solve the subproblem

$$u^{(k)} := \arg\max_{v \in \mathbb{C}_1^n} \; v^* H^{(k)} v$$

  using any convex relaxation, and set $W^{(k)} := u^{(k)} \left(u^{(k)}\right)^*$
- For all $1 \leq i, j \leq n$, find the "peak location" of the spectrogram

$$\hat{\theta}_{ij} := \arg\max_{\phi \in [0, 2\pi]} \left| \mathrm{Re} \left\{ \sum_{k=1}^{k_{\max}} W_{ij}^{(k)} e^{-\iota k \phi} \right\} \right|$$

- Construct Hermitian matrix $\widehat{H} \in \mathbb{C}_1^{n \times n}$ by $\widehat{H}_{ij} = \exp \iota \hat{\theta}_{ij}$, extract the top eigenvector $\tilde{x}$, and perform entrywise normalization to get $\hat{x} \in \mathbb{C}_1^n$

# Why does it work?

- By a perturbation analysis, we expect

$$\widehat{W}^{(k)} = u^{(k)}(u^{(k)})^* = z^k(z^k)^* + E^{(k)} \approx z^k(z^k)^*$$

from solving each subproblem

$$u^{(k)} := \arg\max_{v \in \mathbb{C}_1^n} \; v^* H^{(k)} v$$

- The peak finding step is expected to ensure

$$\begin{aligned}\hat{\theta}_{ij} &= \arg\max_{\phi \in [0,2\pi]} \left| \mathrm{Re}\left\{ \sum_{k=1}^{k_{\max}} W_{ij}^{(k)} e^{-\iota k \phi} \right\} \right| \\ &\approx \arg\max_{\phi \in [0,2\pi]} \left| \mathrm{Re}\left\{ \sum_{k=1}^{k_{\max}} z_i^k \bar{z}_j^k e^{-\iota k \phi} \right\} \right| = \theta_i - \theta_j\end{aligned}$$

provided that $E^{(k)}$ does not "perturb away" the maximum!

# Landscape Analysis of the Dirichlet Kernel

$$2\mathrm{Re}\left\{\sum_{k=1}^{k_{\max}} W_{ij}^{(k)} e^{-\iota k\phi}\right\} = \sum_{k=-k_{\max}}^{k_{\max}} W_{ij}^{(k)} e^{-\iota k\phi}$$

$$= \sum_{k=-k_{\max}}^{k_{\max}} e^{\iota k\left(\theta_i-\theta_j\right)} e^{-\iota k\phi} + \sum_{k=-k_{\max}}^{k_{\max}} E_{ij}^{(k)} e^{-\iota k\phi}$$

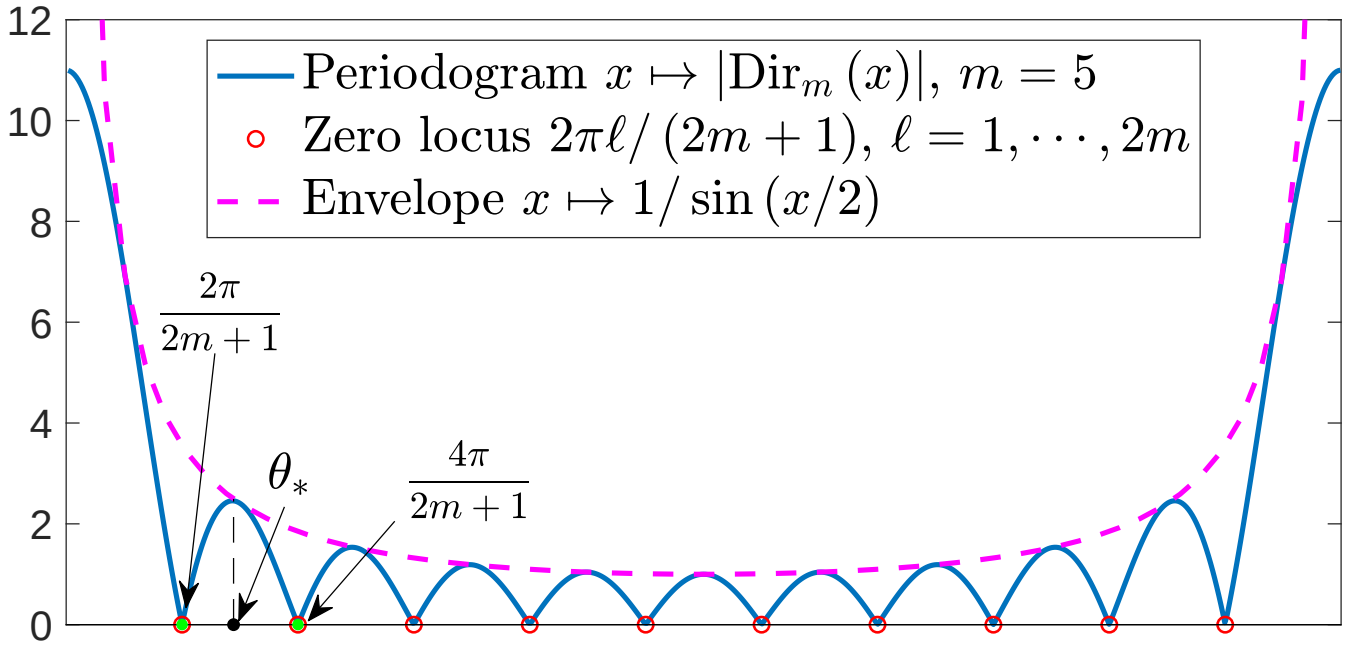
# Landscape Analysis of the Dirichlet Kernel

$$
\begin{aligned}
2\mathrm{Re}\left\{\sum_{k=1}^{k_{\max}} W_{ij}^{(k)} e^{-\iota k\phi}\right\} &= \sum_{k=-k_{\max}}^{k_{\max}} W_{ij}^{(k)} e^{-\iota k\phi} \\
&= \sum_{k=-k_{\max}}^{k_{\max}} e^{\iota k\left(\theta_i-\theta_j\right)} e^{-\iota k\phi} + \sum_{k=-k_{\max}}^{k_{\max}} E_{ij}^{(k)} e^{-\iota k\phi} \\
&= \frac{\sin\left[\left(k_{\max}+\frac{1}{2}\right)\left(\theta_i-\theta_j-\phi\right)\right]}{\sin\left[\frac{1}{2}\left(\theta_i-\theta_j-\phi\right)\right]} + \sum_{k=-k_{\max}}^{k_{\max}} E_{ij}^{(k)} e^{-\iota k\phi} \\
&=: \mathrm{Dir}_{k_{\max}}\left(\theta_i-\theta_j-\phi\right) + R_{k_{\max}}\left(\phi\right)
\end{aligned}
$$

# Landscape Analysis of the Dirichlet Kernel

**Key Observation:** $\left|\hat{\theta}_{ij} - (\theta_i - \theta_j)\right| \leq \theta_* < \frac{4\pi}{2k_{\max}+1}$ whenever

$$2k_{\max} + 1 - R_{k_{\max}}(\phi) > \frac{1}{\sin(\theta_*/2)} + R_{k_{\max}}(\phi)$$



# Landscape Analysis of the Dirichlet Kernel

**Key Observation:** $\left|\hat{\theta}_{ij} - (\theta_i - \theta_j)\right| \leq \theta_* < \frac{4\pi}{2k_{\max}+1}$ whenever

$$2k_{\max} + 1 - R_{k_{\max}}(\phi) > \frac{1}{\sin(\theta_*/2)} + R_{k_{\max}}(\phi)$$

which is satisfied if

$$2k_{\max} + 1 - R_{k_{\max}}(\phi) > \frac{1}{\sin\left(\frac{\pi}{2k_{\max}+1}\right)} + R_{k_{\max}}(\phi)$$

$$\Leftarrow \frac{1}{k_{\max}} \sum_{k=-k_{\max}}^{k_{\max}} E_{ij}^{(k)} e^{-\iota k\phi} = \frac{1}{k_{\max}} R_{k_{\max}}(\phi) < 1 - \frac{1}{2k_{\max}\sin\left(\frac{\pi}{2k_{\max}+1}\right)}$$

**We just need a uniform upper bound for the $E_{ij}^{(k)}$'s!**

# Eigenvector perturbation analysis in $\ell_\infty$-norm!

- Standard perturbation bounds use $\ell_2$-norm (e.g. Davis–Kahan), but most application scenarios of spectral methods require bounding the $\ell_\infty$-norm
- Active research area in recent years, e.g. **[Eldridge et al. (2017)]; [Abbe et al. (2017)]; [Fan et al. (2018)]; [Zhong & Boumal (2018)]**
- Sharpest results to date use a "leave-one-out" trick popularized by statisticians

**Lemma (Gao & Zhao 2019).** For any $0 < \epsilon \leq 2$, with probability at least $1 - O\left(n^{-(2+\epsilon)}\right)$, there exists absolute constant $C > 0$ such that

$$\left\| E_{ij}^{(k)} \right\|_\infty \leq C \sqrt{\frac{\log n}{n}}.$$

• Tingran Gao & Zhizhen Zhao. "Multi-Frequency Phase Synchronization," *The 36th International Conference on Machine Learning* (ICML 2019). arXiv:1901.08235.

# Putting Everything Together

**Theorem (Gao & Zhao 2019).** With all (mild) assumptions satisfied, with high probability the multi-frequency phase synchronization algorithm produces an estimate $\hat{z}$ satisfying

$$\mathrm{Corr}\left(\hat{z}, z\right) \geq 1 - \frac{C'}{k_{\max}^2}$$

provided that

$$k_{\max} > \max\left\{5, \frac{1}{\sqrt{2}\,\pi\left(1 - 4C_2\sigma\sqrt{\log n/n}\right) - 2}\right\}.$$

In particular, $\mathrm{Corr}\left(\hat{z}, z\right) \to 1$ as $k_{\max} \to \infty$.

• Tingran Gao & Zhizhen Zhao. "Multi-Frequency Phase Synchronization," *The 36th International Conference on Machine Learning* (ICML 2019). arXiv:1901.08235.

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# Class Averaging and the Intrinsic Model

- **Goal:** Classify cryo-EM images $I_1, I_2, \ldots$ according to their viewing directions
- **Procedure:**
  - Compute the *rotation-invariant distance* between all pairs of images $d_{\mathrm{RID}}(I_i, I_j) := \min_{\alpha \in [0,2\pi]} \|I_i - e^{\iota\alpha} I_j\|_{\mathrm{F}}$, and denote $\alpha_{ij}$ for the optimal alignment angle
  - Fix threshold $\epsilon > 0$ and define Hermitian $W \in \mathbb{C}^{n \times n}$ by

$$W_{ij} := \begin{cases} \exp(\iota\alpha_{ij}) & \text{if } d_{\mathrm{RID}}(I_i, I_j) < \epsilon \\ 0 & \text{otherwise} \end{cases}$$

  - Solve for the top three eigenvectors of $W$, which embeds $I_1, I_2, \ldots$ into $\mathbb{R}^3$
  - Use correlation in the embedded $\mathbb{R}^3$ space to determine the closeness between viewing directions

# Multi-Frequency Class Averaging

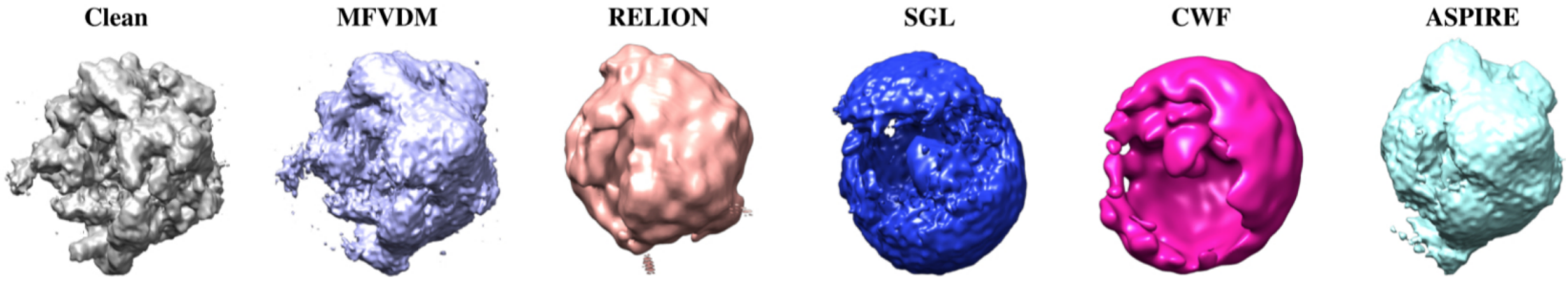
- Idea directly descended from the multi-frequency phase synchronization, but the underlying fibre bundle is non-trivial!
- Fix threshold $\epsilon > 0$ and define for each $k = 1, \ldots, k_{\max}$ Hermitian $W^{(k)} \in \mathbb{C}^{n \times n}$ by

$$W_{ij}^{(k)} := \begin{cases} \exp\left(\iota k \alpha_{ij}\right) & \text{if } d_{\mathrm{RID}}^{(k)}\left(I_i, I_j\right) < \epsilon \\ 0 & \text{otherwise} \end{cases}$$

- Solve for the top $2k+1$ eigenvectors of $W^{(k)}$, which embeds $I_1, I_2, \ldots$ into $\mathbb{R}^{2k+1}$
- Use all correlations in the embedded $\mathbb{R}^{2k+1}$ $(k = 1, \ldots, k_{\max})$ spaces to determine the closeness between viewing directions

• Yifeng Fan & Zhizhen Zhao. "Cryo-Electron Microscopy Image Analysis Using Multi-Frequency Vector Diffusion Maps," *preprint*. arXiv:1904.07772.

# Multi-Frequency Information Improves Class Averaging

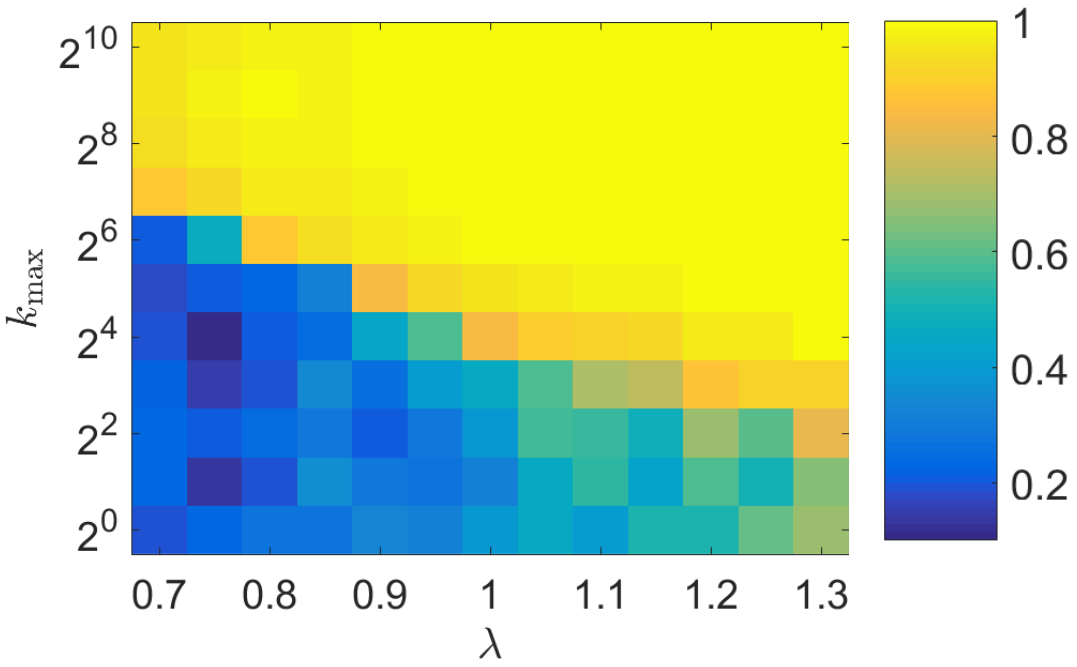



• Yifeng Fan & Zhizhen Zhao. "Cryo-Electron Microscopy Image Analysis Using Multi-Frequency Vector Diffusion Maps," *preprint*. arXiv:1904.07772.

# Open Problems

- Landscape and convergence analysis for the Stage 2 algorithm?
- Algorithm works for $\mathrm{SO}(3)$ seamlessly, but theory?
- Possible extension to other synchronization and multireference alignment problems over compact/noncompact Lie groups?
- Mult-frequency vector diffusion maps?
- A learning paradigm on sheaves?

# Thank You!





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